SUBJECT INDEX

A.E. COSY 128
Al_2O_3
  interaction of V_2O_5 with 499
  interaction of vanadia oxocomplexes with 475
Aldehyde group 26
Alkali metal vanadates 469
$AlPO_4$-based molecular sieves, ^{129}Xe NMR spectroscopy 98
Aluminoborate glasses 221
Aluminosilicate glasses
  chief conclusions made from NMR studies 199
  MAS NMR in 197
  silicon site speciation and coordination of aluminium in 198
  structure of 197
Amorphous III–V semiconductors 269
Amorphous arsenic 268
Amorphous hydrogenated carbon 266
Amorphous hydrogenated germanium 265
Amorphous hydrogenated Si, C:H alloys 266
Amorphous hydrogenated silicon 259
  deuterium NMR studies of α-Si:D 265
  films 259
  hydrogen environments 261
  isovalent substitution in α-Si:H 265
  spatial distribution of hydrogen 262
  spin-lattice relaxation by molecular hydrogen 262
Amorphous hydrogenated silicon carbide 266
Amorphous intermetallic systems 277
Amorphous metal hydrides 273
Amorphous metal–metalloid systems 273
Amorphous phosphorus 268
Amorphous silicon nitride 268
Arsenic chalcogenide glasses 246

^{11}B NMR 216
β-radiation detected NMR 542
Bloembergen–Purcell–Pound (BPP) description of relaxation rate 529
Borate glasses 215
  alkali and alkaline-earth aluminoborate glasses 221
  binary alkali 218
  further NMR studies 222
  intermediate range order in alkali 220
  network modification by intermediate oxides 221
  network structure in binary alkali 216
  short and intermediate range order in glassy B_2O_3 215
  short range order and its analysis via ^{11}B NMR 216
Boron chalcogenide glasses 236, 247
Borophosphate glasses 228
Borosilicate glasses 232
Brain, ^{23}Na MRI 423–5

^{13}C NMR 447
  assignment of spectra 2
  coupling constants 4
  derivatization 5
  determination of carbon type 2
  isotopic labelling 6
  oleanane triterpenoids. *See* Oleanane triterpenoids
  shift reagents 4
  solvent effects 4
CAMELSPIN 378
Carbon–hydrogen coupling constants 4
Carboxylic group 27
Cartilage, ^{23}Na MRI 424
(^{13}C,^{2}H) case 453
Chalcogenide glasses
  atomic distribution in binary and ternary III, IV, and V 236
  competitive network modification 252
  effect of Al_2S_3 252
  effect of B_2S_3 254
  effect of SiS_2 252
  non-oxide 235
  site speciation in binary and ternary III, IV, and V 236
  site speciation in network former/network modifier systems 247
Chemical shift anisotropy (CSA)
  interactions 379, 382, 383, 403
  parameters 470
  relaxation 382, 389, 403
Chemical shift correlation spectroscopy 185
Chemical shift imaging 412, 420, 422
Chemical shift interaction 170
Clustering in solids 323
(^{13}C,^{14}N) pair 447
Cobalt borides 274
Cobalt phosphides 274
Continuous random network model 165
Correlated external random magnetic fields 367
COSY 110
CRAMP techniques 453
Cross-polarization (CP) 184
Cyclooleananes 50, 68

Density matrix 383
  basis sets 387
DEPT 329, 348, 350, 393
Differential scanning calorimetry (DSC) of glasses 164

Diffusion-controlled relaxation (DCR) model 534
Diffusion studies 365
Dipolar coupled spectra 328
Dipolar spin-echo double resonance spectroscopy 183
Dipolar spin-echo NMR 182
Dipole dipole relaxation 390, 403
Distance geometry (DG) 146
DNA
  backbone torsion angles 138
  structure and function in living cell 109
  structure determination 110
DNA segments
  cross peaks and coupling constants in spectra of 118
  J-correlated spectra 119
Double quantum correlation experiments
  abundant nuclei 340
  automated spectral analysis 341
Double quantum (DQ) spectra 124
Double quantum filtered (DQF) COSY 124
Double rotation (DOR) 182
Dynamic angle spinning (DAS) 182
Dynamic N ↔ S equilibria 129

E. COSY 128, 319
EFG tensor 443, 448
Electric field gradient (EFG) 437
Eyes, ^{23}Na MRI 423, 427

Fluorinated amorphous silicon 265
Four-dimensional correlation experiments 354
Fourier imaging 418, 421
Free induction decay (FID) 119, 187, 415, 428
Friedooleananes 68
  ^{13}C NMR chemical shifts 55
  substitution pattern 24

GaAs 269
Gallium oxide based glasses 234
GaP 269
Germanium–silicon alloys 265
Glasses 164
  differential scanning calorimetry (DSC) 164
  magic angle spinning (MAS) technique 544
  quantitative NMR spectroscopy 186
Glassy solid electrolytes, ionic diffusion studies 254
Gradient echoes 415, 421
Gyromagnetic ratio 167

^{1}H–^{13}C correlated spectroscopy 8
^{1}H–$_{1}$H correlated spectroscopy 7
^{1}H–^{1}H coupling constants, sugar geometries from 135
^{1}H–^{31}P heteronuclear coupling constants 138
Halide glasses 234
Hartmann–Hahn condition 185
Heart, ^{23}Na MRI 422, 425, 426
Heteronuclear 3D and 4D experiments 356, 358
Heteronuclear editing 329
Heteronuclear multiple-quantum chemical shift 347
High-pressure NMR studies, superionic conductors (SIC) 541
HMQC experiment 323, 348, 350, 351
HMQC module 355
HMQC–COSY experiment 351
HMQC–HOHAHA experiment 352
HMQC–NOESY experiment 352
Homonuclear editing 335
Hydrogenated amorphous silicon
  local structure of dopants in 267
  silicon speciation and bond angle distributions 260
Hydrogenated boron nitride films 268
Hydroxyl groups 23

INADEQUATE 8, 313, 339
INEPT 393
Initial rate approximation (IRA) 146
Inter-residue scalar coupling correlation 358
Ionic diffusion studies of glassy solid electrolytes 254
Ionic glass systems 234
Iron borides 273
Isolated spin pair approximation (ISPA) 146

J-correlated spectra 114
J-coupling 110
Jump-relaxation model 532, 535

Knight shift 170
Kohlrausch–Williams–Watts (KWW) function 530
k-space formalism 416
$K_3V_5O_{14}$ 469
KVO_3
  ^{51}V NMR spectra 514
  calculated spectra 467
  computer simulated spectra 459
  experimental and calculated spectra 459, 460
KVO_3–$K_2S_2O_7$ alloys 510
  at low S/V ratio 516

Li_2S–P_2S_5 system 249
Liquids, relaxation in rotating frame 377
Locally ordered random packing model 166
Lungs, ^{23}Na MRI 425

Magic-angle spinning (MAS) 181, 435
  glasses 544
Magnetic dipole–dipole interaction 172, 381
Magnetic field gradients 359, 414, 417
Magnetic resonance imaging (MRI) 412
Magnetic resonance techniques 414
MAS-NMR 181, 184, 187
Metal clusters in porous materials, ^{129}Xe NMR spectroscopy 101
Metal–metalloid systems 277
Metallic glasses 272
Metavanadates 469, 473
Microporous solids, ^{129}Xe NMR spectroscopy 91
Microscopic activation energy 535

MINSY experiment 387, 408
Multiple-quantum coherence 296
  chemical shift and sensitivity to magnetic field gradients 300
  coherence order 300
  evolution 304
  excitation and detection 305, 311
  inhomogeneous *z*-pulses 302
  magnetic field gradients 302
  manipulation 301
  non-selective pulse techniques for excitation in liquids 307
  phase cycling 301
  precessional frequency 300
  properties of 300
  pulse angle effects 303
  relaxation-generated 322
  relaxation properties 366
  scalar and dipolar couplings 301
  selective single-quantum pulses 305
  sensitivity to radio frequency pulse phase shifts 301
  uniform excitation 307
Multiple-quantum filtered experiments 323
  COSY 316
  NOESY 322
Multiple-quantum filtration and relaxation 320
Multiple-quantum NMR methods 295
  chemical shift 338
  models and formalisms 297
  number of active spins 313
  operator formalisms 298
  physical picture 297
  principles of 297
  sensitivity to magnetic field gradients 359
Multiple-quantum pulses 305
Multiple-quantum relaxation times 366
Multiple quantum spectroscopy (MQSY) 110

^{23}Na chemical shift imaging 411, 430
^{23}Na MRI 411, 412
  addition of contrast agents 429
  applications 422
  calculation of sodium concentrations and relaxation times 425
  eyes 423, 427
  heart 422, 425, 426
  lungs 425
  specific techniques 421
  tissue contrast 424
  tumors 424, 428
Nernst–Einstein equation 533
NH_4VO_3, ^{51}V MAS spectrum 461
Nickel borides 275
Nickel phosphides 275
NMR Hamiltonian 167
NMR imaging 364, 377
  superionic conductors (SIC) 539
NMR lineshape 167, 170, 172, 174, 176
  temperature-dependent studies 254
NMR powder patterns 171
NMR relaxation 366
NMR resonance frequencies 167
NMR studies of superionic conductors (SIC) 527
NOESY experiment 110, 186, 387, 393
Noncrystalline solids 164
Non-oxide chalcogenide glasses 235
Noroleananes 68
n-spin filtration 335
Nuclear electric quadrupole interaction 173
Nuclear Overhauser enhancement (NOE) 110
  in multispin systems 146
  simulation of correlated spectra 146
Nuclear Overhauser enhancement difference spectroscopy (NOEDS) 9
Nucleic acids, solution conformations of 109

^{17}O NMR spectra
  pyrosulfates of alkali metals 515
  V_2O_5–$K_2S_2O_7$ samples in molten state 515
Oleanane glycosides 70
Oleanane triterpenoids 1–90
  ^{13}C NMR chemical shifts 28, 61
    related to oleanolides and cyclooleananes 50
  ^{13}C NMR shielding behaviour 9
  chemical shift (ppm) increments 63
  index of 78
  parent skeleton of 3, 63
  substitution pattern 10
    related to oleanolides, cyclooleananes and noroleananes 20
Oleananes 9, 70
Oleanolides 50
Oleanoloids 27
Olefinic bond 22
ω_1-decoupled COSY 128
One-dimensional DOUBTFUL 338
One-dimensional INADEQUATE 313
One-dimensional multiple-quantum filtration 314
Orthovanadates of divalent metals 471
Oxide glass conformer systems 226
Oxidooleananes 68
Oxo-group 26
Oxoselenatovanadates (V) of alkali metals 505, 507
Oxosulfatovanadates (V) of alkali metals 505

Pachysanane 69
P.E. COSY 128
Perturbation theory 437
Phosphate glasses 223
  anion substitution 224
  coordination of other glass constituents in 226
  network structure in binary and pseudobinary 223
Phosphorous chalcogenide glasses 238
Phosphorus–selenium based ternary systems 244
Phosphorus–selenium system 238
Phosphorus–sulfur system 246
Phosphosilicate glasses 226
Plasma-enhanced chemical vapor deposition (PECVD) 259
Pnictide glasses 270

Polymer electrolytes 546
POMMIE 323, 332
Potassium vanadate 469
Principal axis system (PAS) 443
Product operators 383
Projection reconstruction 418, 421
Pulsed-field gradient (PFG) method 535
Pulsed NMR experiments 178
Pyrosulfates of alkali metals 515
Pyrovanadates of divalent metals 471

Quadrupolar coupling 326
Quadrupolar nuclei 435
Quadrupolar relaxation 367
Quadrupolar resonance frequency 175
Quantitative NMR spectroscopy in glasses 186

Radial distribution function (RDF) measurements 260
Radio frequency (RF) magnetic fields 377
  strong 387, 390
  weak 389
Random close-packing model 166
Random coil model 166
Rapid exchange model 104
REDOR (rotational spin echo double resonance) 184
Relative transverse relaxation rates 352
Relaxation
  and multiple-quantum filtration 320
  as constraint 369
  effect of secular and non-secular terms in 386
  in rotating frame in liquids 377
  multiple-quantum coherence 366
  selection rules 385
Relaxation equation 379
Relaxation-generated multiple-quantum coherence 322
Relaxation matrices 394
RELAY 323
Resonance offset effects 405
Restrained molecular dynamics (RMD) 146
Reverse detection experiments 350
ROESY experiment 378, 381, 386, 405, 408
RRR (rotary resonance recoupling) 184

Scalar coupled spectra 327
Scalar relaxation 368
^{77}Se NMR MAS spectra of oxoselenatovanadates (V) of alkali metals 507
Selective averaging techniques 181
SEMINA 333
SHARP 364
SICOS program 119
Silica supported rhodium catalysts 487
Silicate glasses 187
  and melt structure at high pressures 204
  and melt structure at high temperatures 202
  anion substitution 200
  bond angle distribution in vitreous SiO_2 187
  hydrogen bond strength characteristics 207
  identification and quantification of hydrous environments 211
  interaction of water with silicate melts and glasses 206
  interaction with water at low temperatures 210
  motional properties 209
  network structure 190
    and hydrogen environments in sol–gel prepared glasses and amorphous silicas 210
    of sol–gel derived silicas and silicate glasses 213
  $Si^{(n)}$ sites formation and analysis by ^{29}Si NMR 190
  $Si^{(n)}$ speciation of M_2O–SiO_2 glasses 195
  $Si^{(n)}$ species distribution and cation clustering
    in alkaline earth 196
    in binary alkaline 192
  speciation of water 206
  structural characteristics of hydrous species 206
Silicon chalcogenide glasses 236
Simulated annealing (SA) 146
Simulation software packages 152
Single-quantum chemical shift 348
SLAP 333
SL-ROESY experiments 386
(^{119}Sn,$^{35/37}$Cl) pair 451
SO_2 oxidation
  interaction of active component of vanadia catalysts with support 512
  vanadia catalysts for 505
  vanadia complexes in 519
  vanadium catalysts of 518
Sol–gel derived silicas 213
Sol–gel process 210
Solid state ionics 527
  NMR problems in 529
Solid state NMR 159
  fundamentals of 167
  historical background 162
  studies of glasses 161, 163
Solution conformations of nucleic acids 109
Spectral densities 381, 394
Spin echo double resonance (SEDOR) 183
Spin echoes 415, 421
Spin–lattice interaction 382
Spin–lattice relaxation 176, 533, 534
Spin–lattice relaxation times 180
  temperature-dependent 256
Spin-½ magic-angle spinning spectra of solids 435
  applications 447
  (^{13}C,^{2}H) case 453
  (^{13}C,^{14}N) pair 447
  coupling to same quadrupolar nucleus 444
  coupling to several quadrupolar nuclei 444
  miscellaneous cases 453
  ^{31}P interacting with metals 452
  quadrupolar effects transferred to 435
  self-decoupling 446
  (^{119}Sn,$^{35/37}$Cl) pair 451

theory 437
use of spinning sidebands 446
variable-angle experiments 446
Spin operators 381
Spin order, changes in 385
Spin topology filtration 335
Sugar geometries from ^{1}H–^{1}H coupling constants 135
Sugar ring patterns for single conformation 121
Superionic conductors (SIC)
beta-radiation detected NMR 542
coupling model 530
crystalline solids 543
diffusion-controlled relaxation (DCR) model 534
experimental techniques 535–43
general properties of 528
high-pressure NMR studies 541
jump-relaxation model 532, 535
NMR studies 527, 529, 539
pulsed-field gradient (PFG) method 535
studies of special substances 543
two-level systems 532

Taraxerane triterpenoids
^{13}C NMR chemical shifts 54
substitution pattern 23
Taraxeranes 68
Tellurium oxide based glasses 234
Thiosilicate glasses 248
Three-dimensional correlation experiments 354
Three-dimensional imaging 419
TiO_2
interaction of V_2O_5 with 499
vanadia complexes 494
Titania promoted vanadia catalysts 487
$TmDOTP^{5-}$ 430
TOCSY/HOHAHA magnetization transfer 387, 406, 407
Total spin coherence transfer echos 362
Triple quantum filtered, tilted frame ROESY (3QF-T-ROESY) experiment 386
Tumors, ^{23}Na MRI 424, 428
Two-dimensional correlated spectroscopy (COSY) 185
Two-dimensional heteronuclear correlation experiments 346
Two-dimensional homonuclear correlation spectroscopy 338
Two-dimensional INADEQUATE 8, 339
Two-dimensional NMR 418
Two-dimensional NMR spectra, simulation of 109
Two-dimensional NMR spectroscopy 7
Two-dimensional nuclear Overhauser effect spectroscopy 9

Ultra-high intensity grinding (UHIG) 499
UNCOSY 323

^{51}V NMR chemical shift parameters 463
^{51}V NMR MAS spectra, calculated and experimental 464
^{51}V NMR parameters, inter-relation with local environment of V nuclei 462
^{51}V NMR spectra
computer simulation 461
in high magnetic fields 463
of industrial catalysts 512
of KVO_3–$K_2S_2O_7$ systems 510, 516
of molten V_2O_5 and KVO_3 514
of oxoselenatovanadates (V) of alkali metals 505
of oxosulfatovanadates (V) of alkali metals 505
of solids 458
of V_2O_5–$K_2S_2O_7$ alloys 510
of V_2O_5–K_2SO_4 systems 516
solids with well characterized structures 462
^{51}V solid-state NMR studies of vanadia-based catalysts 457
Vanadates
of divalent metals 470
of monovalent metals 468
of trivalent metals 473
Vanadia catalysts 475
SO_2 oxidation 505, 512
^{51}V solid-state NMR studies 457
Vanadia complexes
in V_2O_5/MgO catalysts 492
on SiO_2 483
on SnO_2 498
on TiO_2 494
on ZrO_2 498
SO_2 oxidation 518, 519
Vanadia oxocomplexes, interaction with Al_2O_3 surfaces 475
Vanadium catalysts for SO_2 oxidation 518
V_2O_5
calculated spectrum 461
computer simulated spectra 459
experimental spectra 461
interaction with Al_2O_3 499
interaction with TiO_2 499
^{51}V NMR spectra 514
V_2O_5/$AlPO_4$ catalysts 482
Vogel–Tammann–Fulcher (VTF) equation 547
V_2O_5–$K_2S_2O_7$ alloys 510
in molten state 515
V_2O_5–K_2SO_4 systems at low S/V ratio 516
V_2O_5/(TiO_2–ZrO_2) catalysts 497

^{129}Xe chemical shift, correlation of pore dimensions with 103
^{129}Xe NMR spectroscopy
$AlPO_4$-based molecular sieves 98
historical background 91
low temperature 105
metal clusters in porous materials 101
microporous solids 91
miscellaneous applications 100

Zeeman interaction 167
Zeeman-perturbed NQR 176
Zeeman-quadrupole Hamiltonian 437
Zeolites
  molecular sieves 92
    with one possible adsorption zone 92
    with two or more possible adsorption zones 96
Zero-quantum coherence 343
z-filtered double-quantum experiment 343